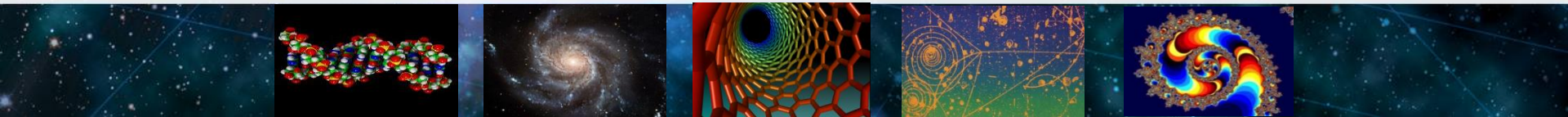
Mathematical and Physical Sciences Advisory Committee (MPS AC)

F. Fleming Crim

Assistant Director

April 3, 2014



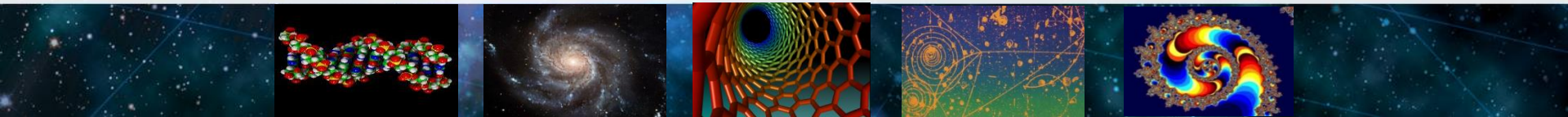
Ab Initio Prediction of Molecular Crystal Structures

A Science Hors d'Oeuvre

Ab Initio Prediction of Molecular Crystal Structures

"One of the continuing scandals in the physical sciences is that it remains in general impossible to predict the structure of even the simplest crystalline solids from … their chemical composition."

John Maddox, *Nature*, 1988



Ab Initio Prediction of Molecular Crystal Structures

Polymorphs

Multiple arrangements of molecules in a crystal of the same compound, which often differ only slightly (1 – 10 kJ/mol) in energy.

Bioavailability and stability of pharmaceuticals

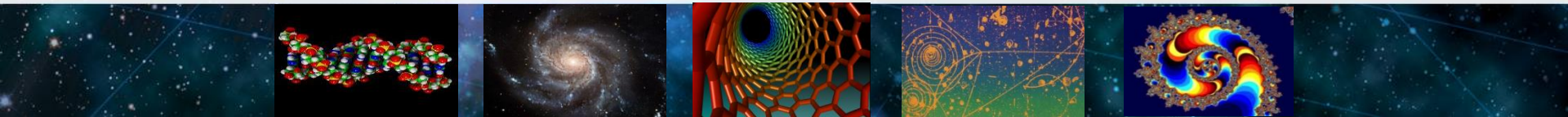
$ 250 M recall of HIV drug Ritonavir

Phases of ice and other compounds

Metastable phase V

Stable phase VI

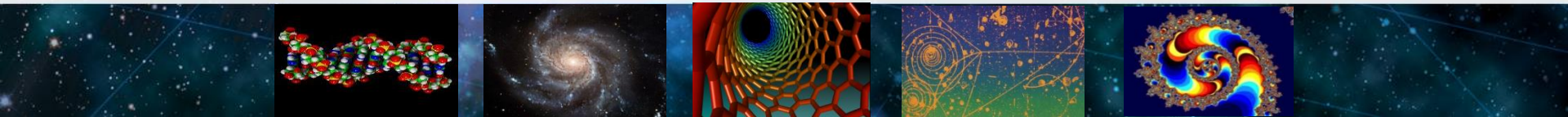
K. Roth,
Chem. Unser Zeit, **39**, 416 (2005)



Ab Initio Prediction of Molecular Crystal Structures

Greg Beran
University of California,
Riverside

So Hirata
University of Illinois
at Urbana-Champaign



Ab Initio Prediction of Molecular Crystal Structures

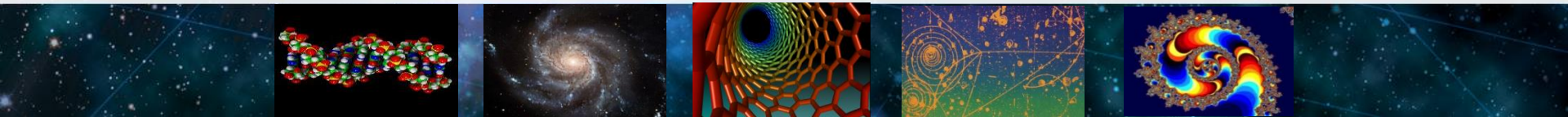
Polymorphs in molecular crystals
(asprin, oxalyl dihydrazide, …)

Greg Beran
University of California,
Riverside

Both work on structures of ice and
both collaborate with experimentalists

So Hirata
University of Illinois
at Urbana-Champaign

Spectra and phase transitions
(solid-solid transition in CO_2, …)



Ab Initio Prediction of Molecular Crystal Structures

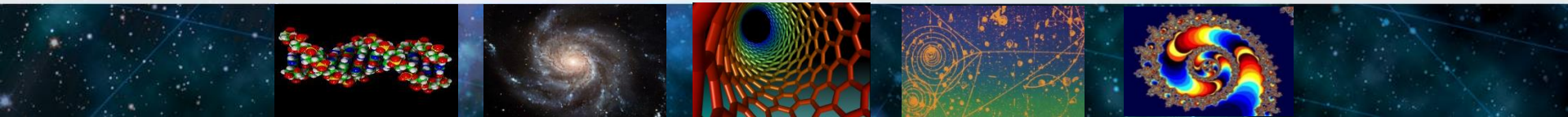
Quantum mechanics-
Molecular mechanics methods
(QM/MM)

Greg Beran
University of California,
Riverside

"Fragment methods"
model the interplay of weak forces
that determine the structure of a
molecular crystal

So Hirata
University of Illinois
at Urbana-Champaign

Fragments embedded in crystal's
electrostatic environment



Ab Initio Prediction of Molecular Crystal Structures

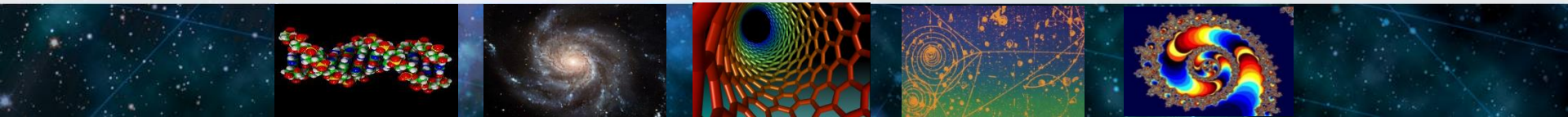
XSEDE
Extreme Science and Engineering Discovery Environment

Greg Beran
University of California, Riverside

NSF

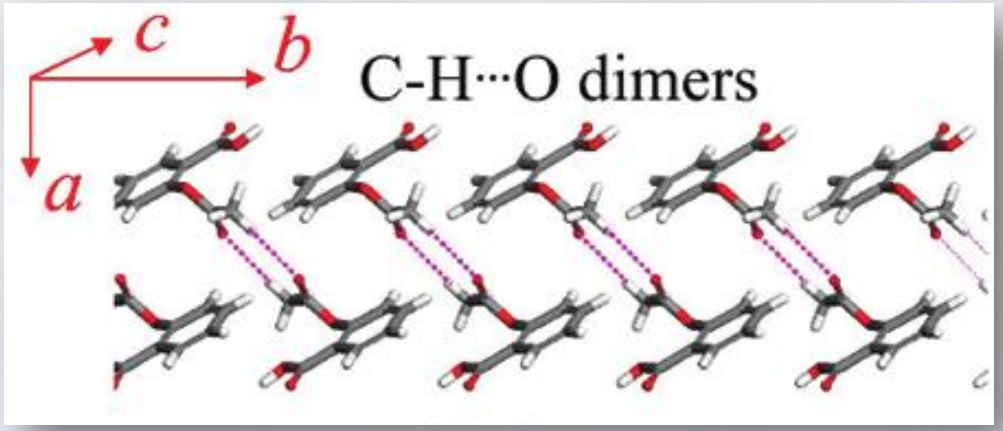
Advances in computer power, computational methods, and algorithms enable this research

So Hirata
University of Illinois at Urbana-Champaign

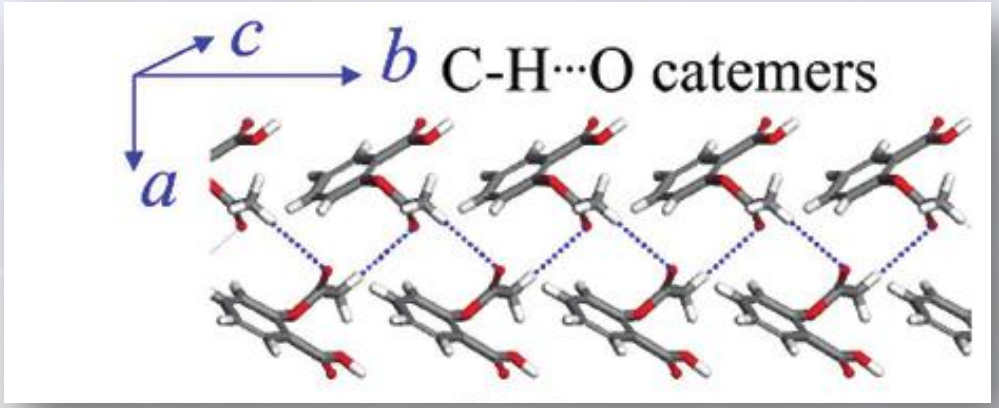


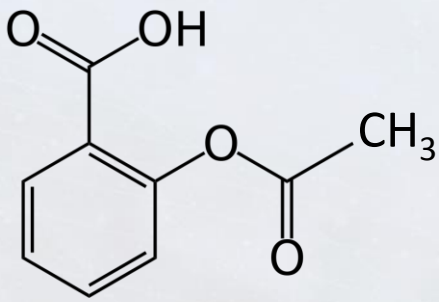
Ab Initio Prediction of Molecular Crystal Structures

Polymorphs of Asprin

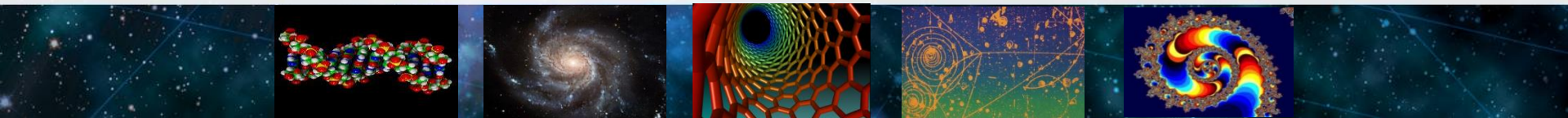


Greg Beran





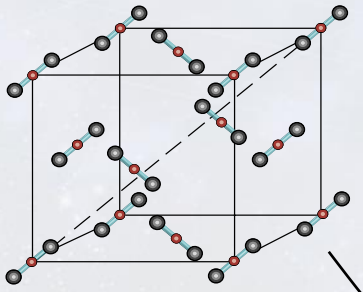
Wen and Beran, Crystal Growth and Design 2012, 12, 2169



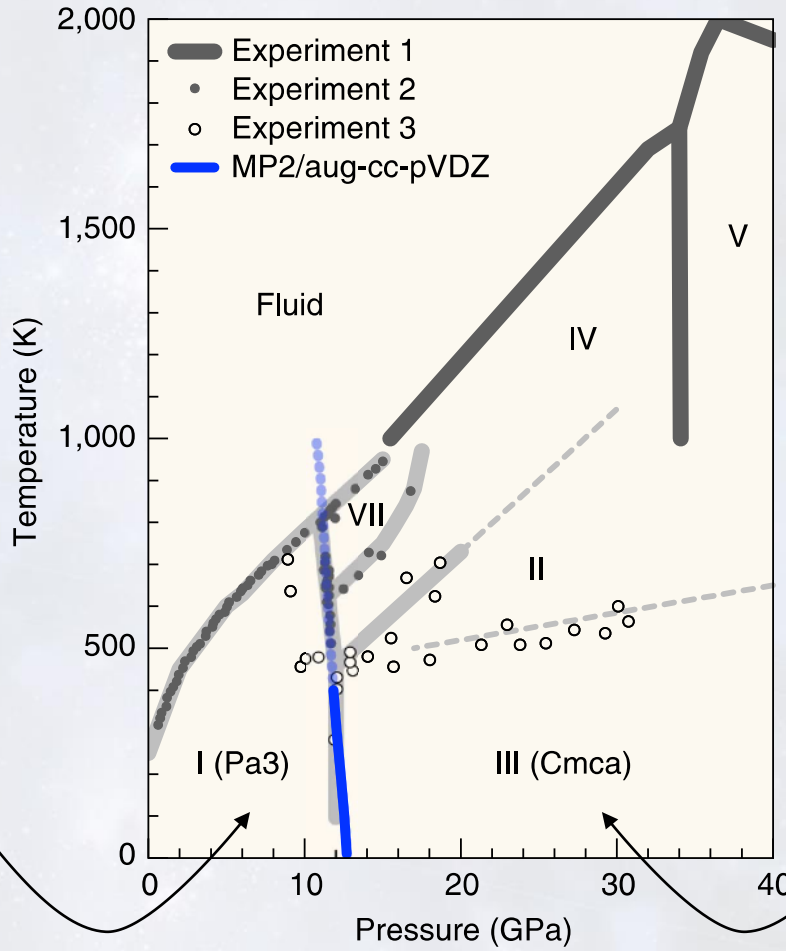
Ab Initio Prediction of Molecular Crystal Structures

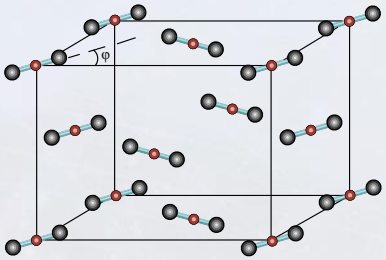
Phase Diagram of CO_2

So Hirata



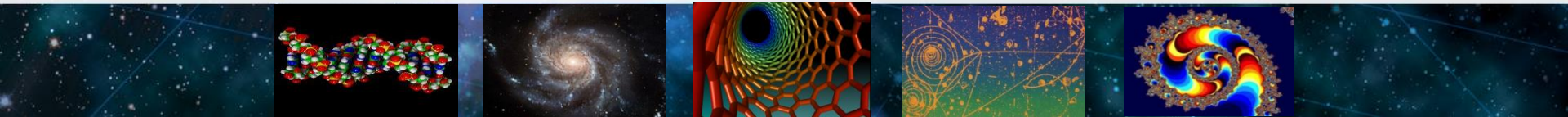
I(Pa3)





III(Cmca)

Sode, Voth, Hirata, Nature Communications 2013, 4, 2647

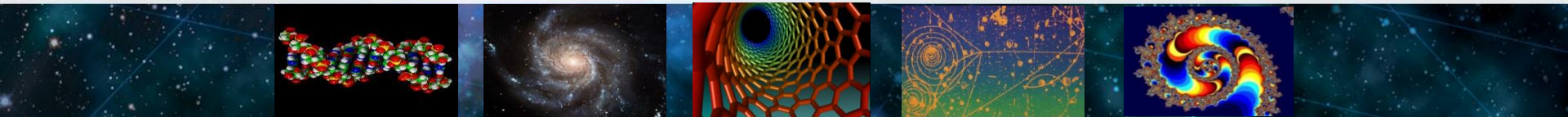


Ab Initio Prediction of Molecular Crystal Structures

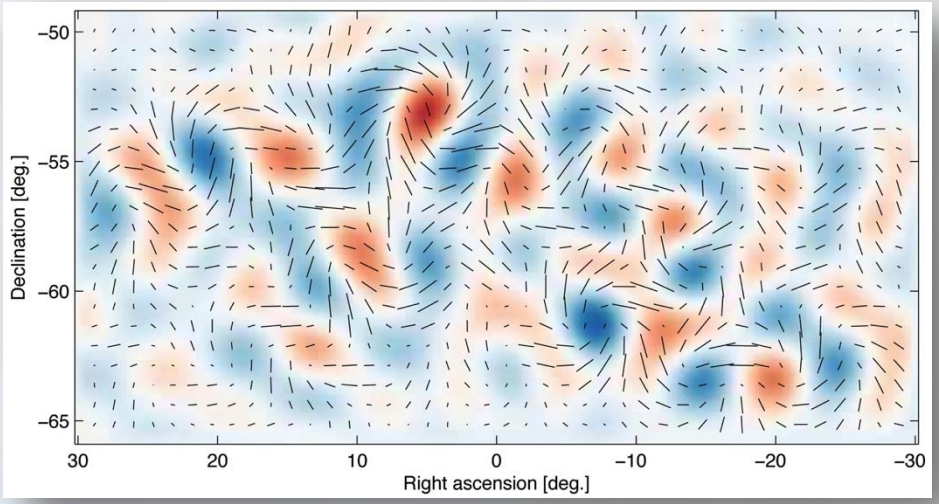
Greg Beran
University of California,
Riverside

So Hirata
University of Illinois
at Urbana-Champaign

Thanks to Evi Goldfield

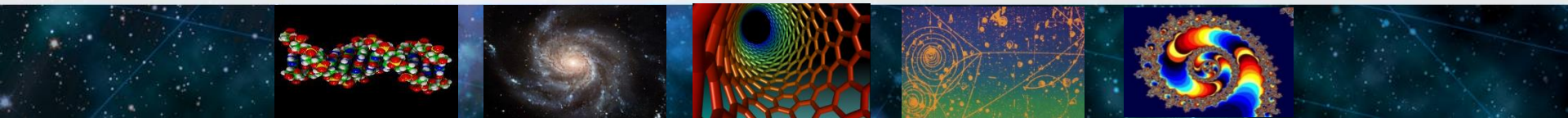


A Multi-Directorate Lagniappe (GEO, MPS, CISE)



"Thank you to the **Office of Polar Programs**, particularly to **Kelly, Scott, Brian, and Vladimir**, for your tireless championing of world-class science at the ends of the world. I also owe great thanks to those of you throughout NSF, particularly **Nigel Sharp, Richard Barvainis, Jim Whitmore, Dan Katz** and your colleagues at **AST, PHY, and ACI** who have championed our interdisciplinary efforts and been willing **to work across unit boundaries to support the best science wherever it is in the world."**

John Kovac, Astronomy Department, Harvard



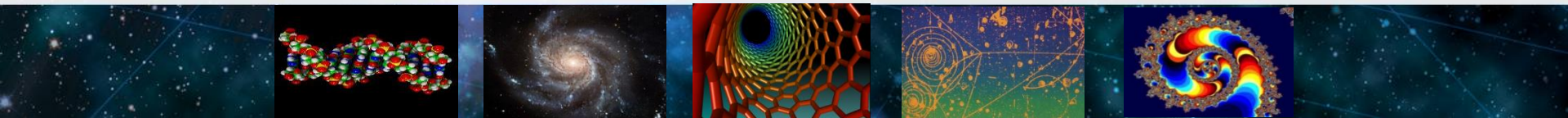
Personnel and Plans

Budget

Facilities

Program Updates

Agenda

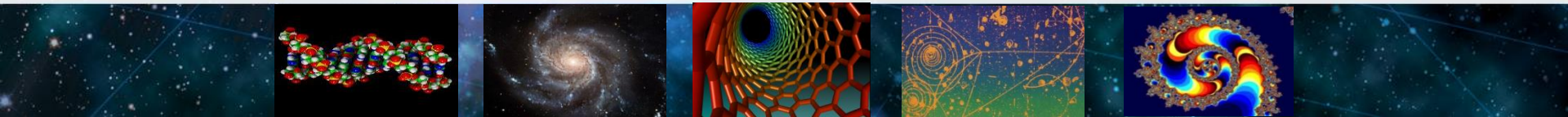


MPS Advisory Committee

Quarterly Meetings

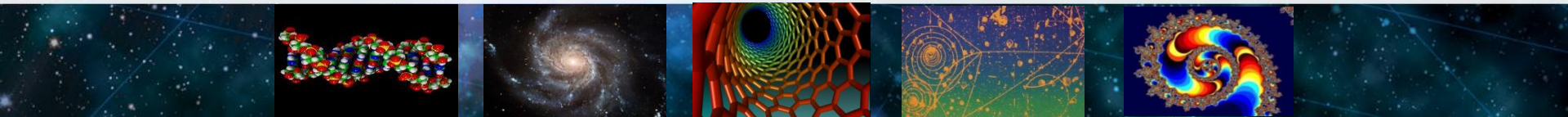
(3 virtual, 1 at NSF)

Next Meeting (virtual)
July 18, 2014



New Home for NSF
(2017)

Alexandria, VA

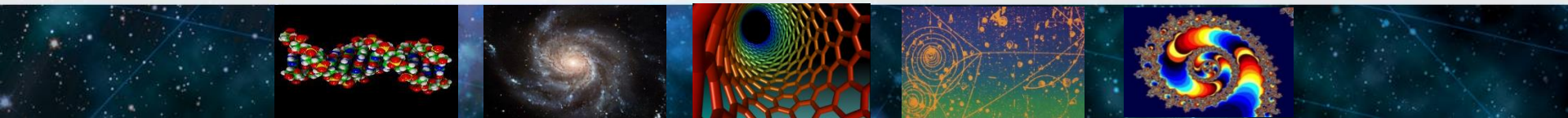


New Accounting System for NSF (October, 2014)

Commercial, off-the-shelf product
Real-time status information
Increased financial and process controls

Requires an early closeout in FY 2014 and a late start to FY 2015
- not a shutdown, open for business -

Part of continuing modernization of
proposal submission, management and review, post-award functions



Personnel and Plans

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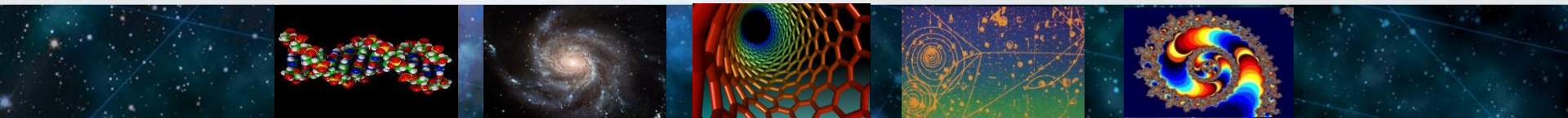
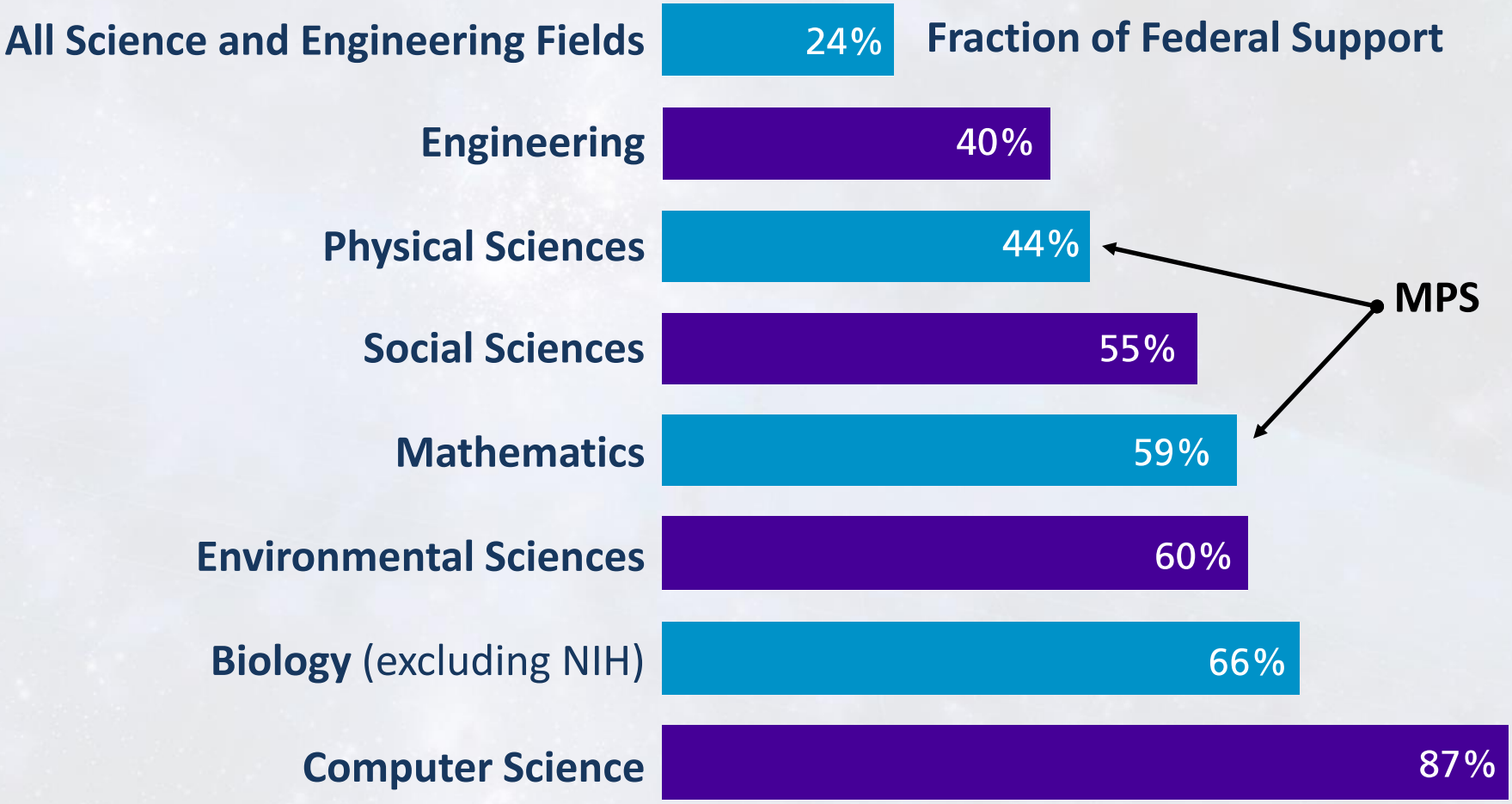
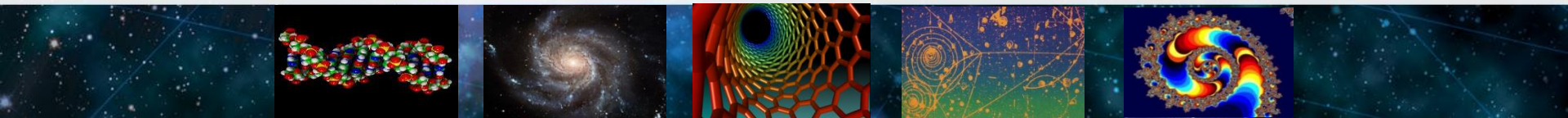
FY 2015 "Roll out"
March 10, 2014



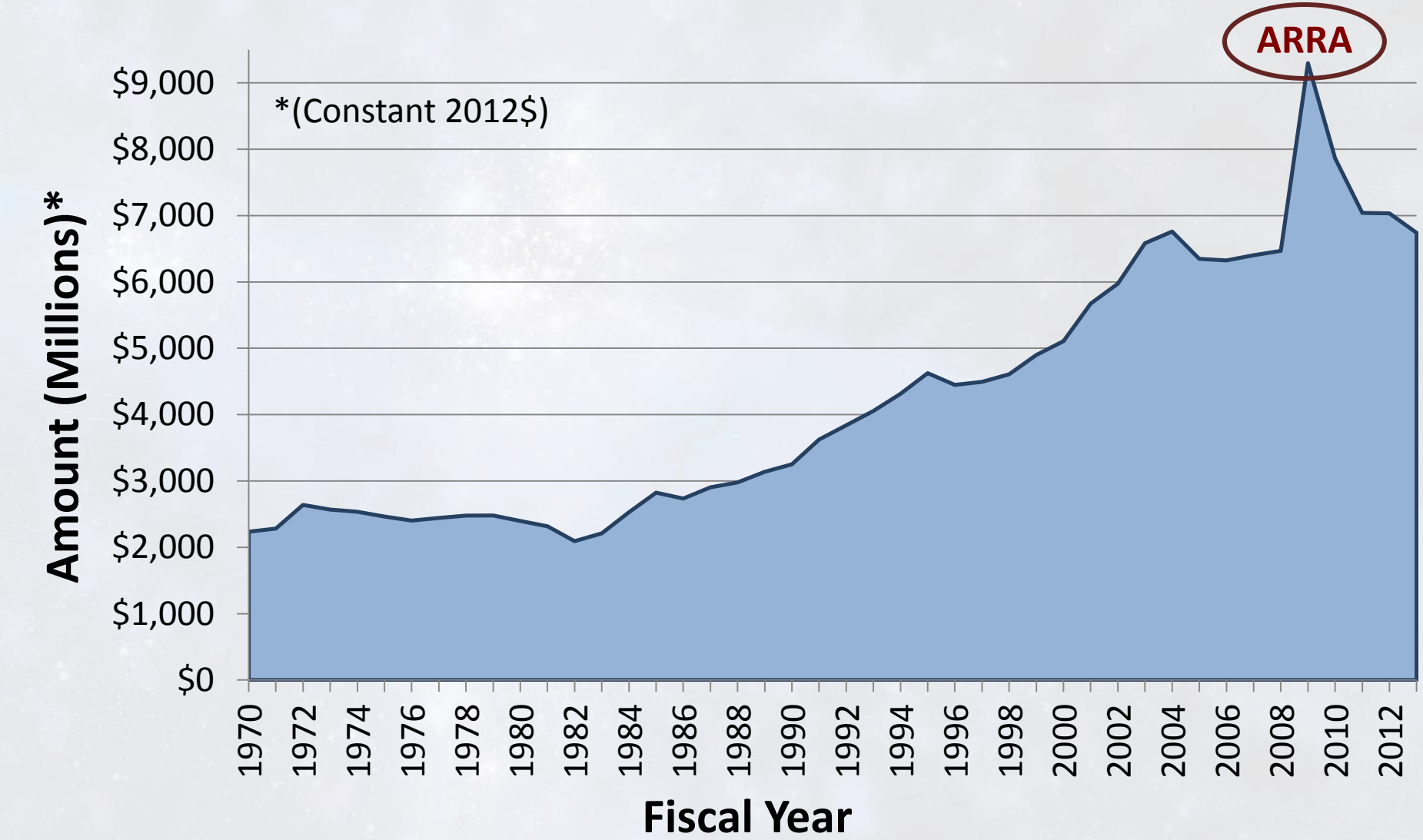
NSF Supports Academic Basic Research

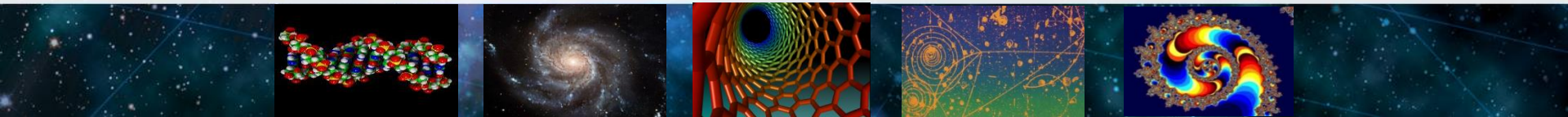


Source: NSF/ Center for National Science and Engineering Statistics, FY 2011

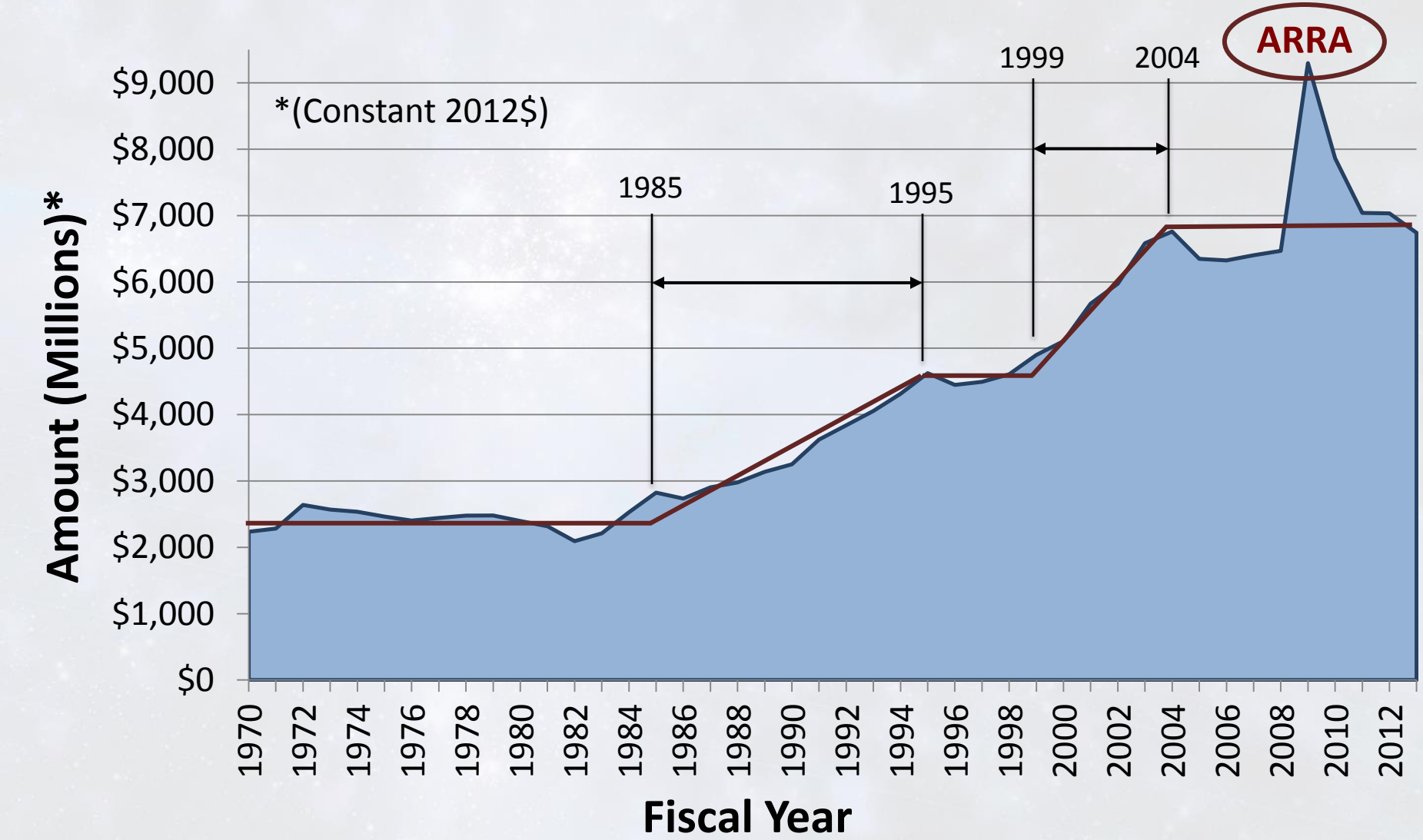


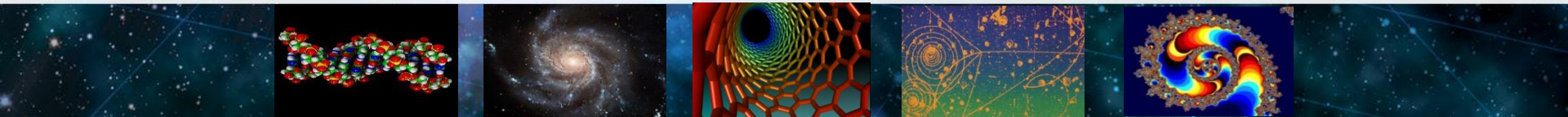
NSF Funding History





NSF Funding History

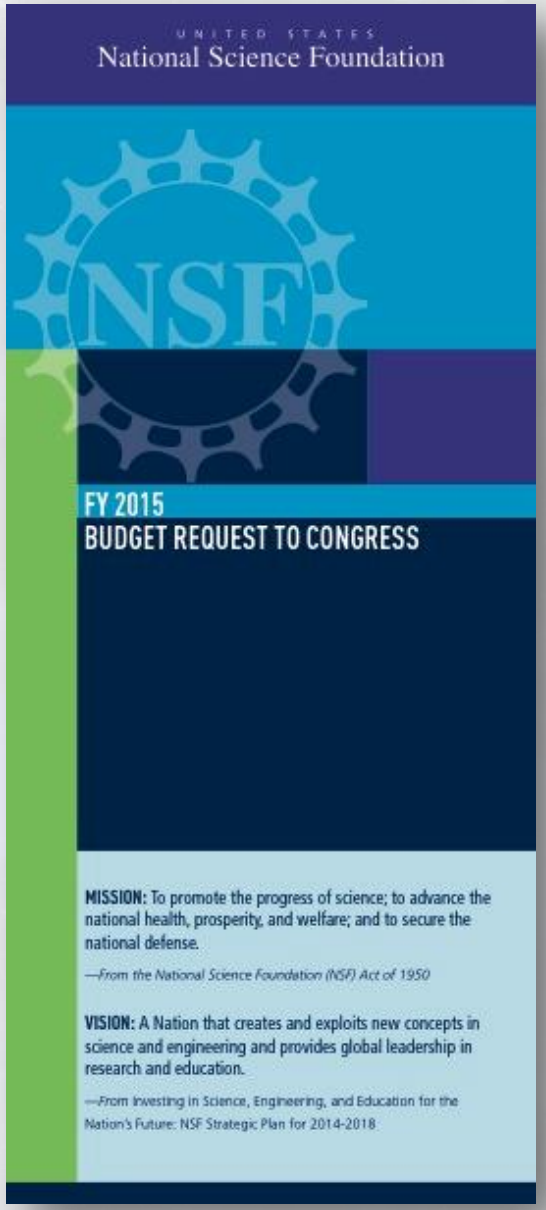


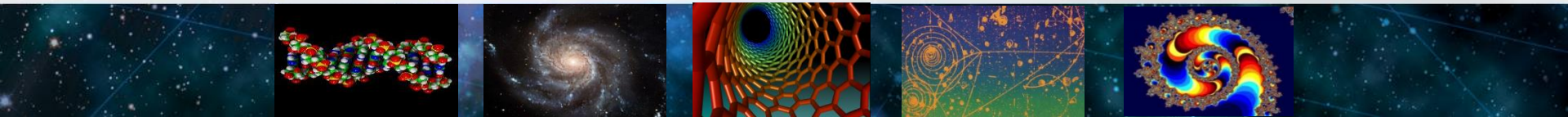


UNITED STATES
National Science Foundation

	FY 2014 (estimate)	FY 2015 (request)	
NSF	$ 7172 M	$ 7255 M	1.2%
R&RA	$ 5808 M	$ 5807 M	--

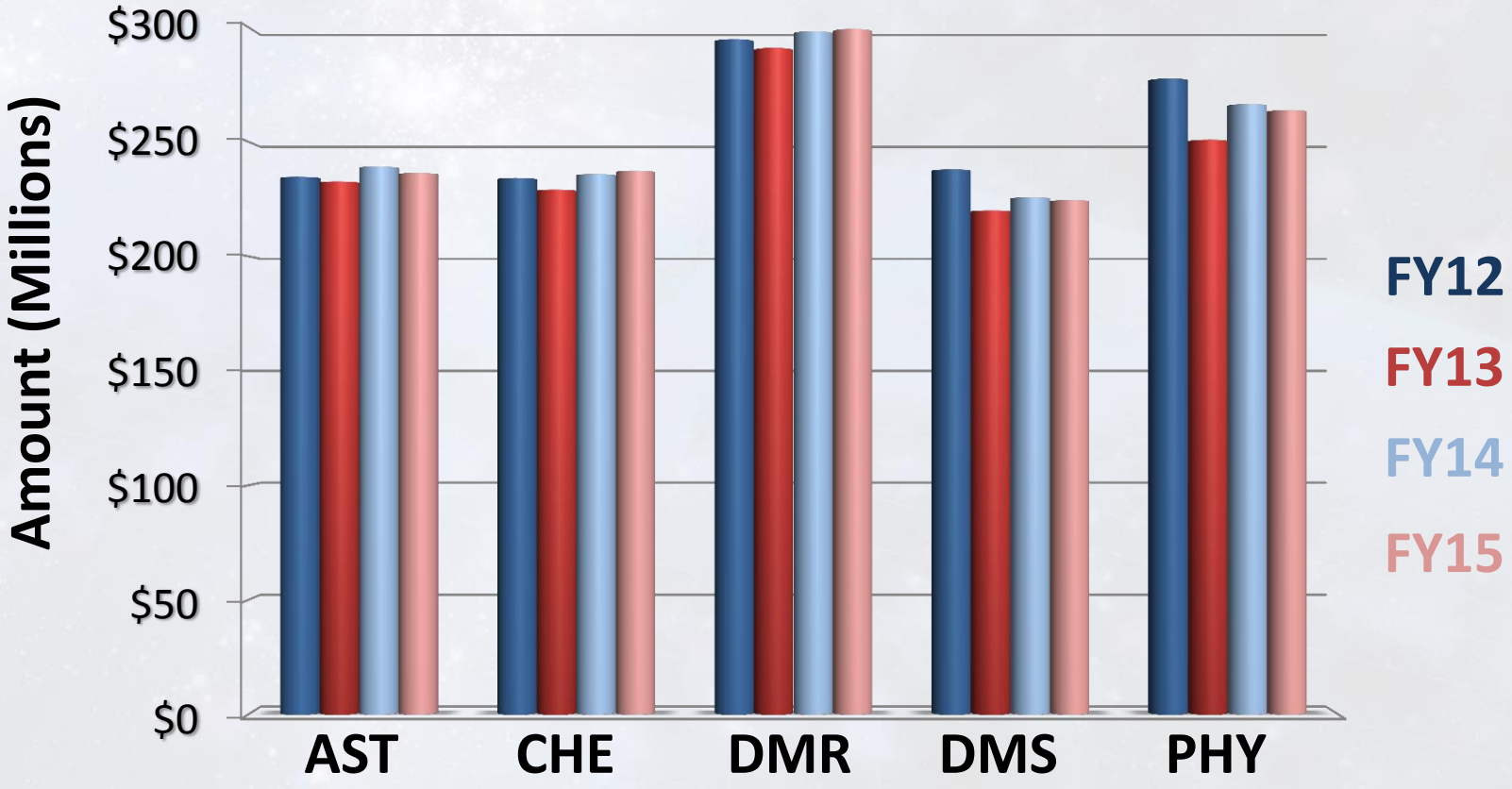
FY 2015
BUDGET REQUEST TO CONGRESS



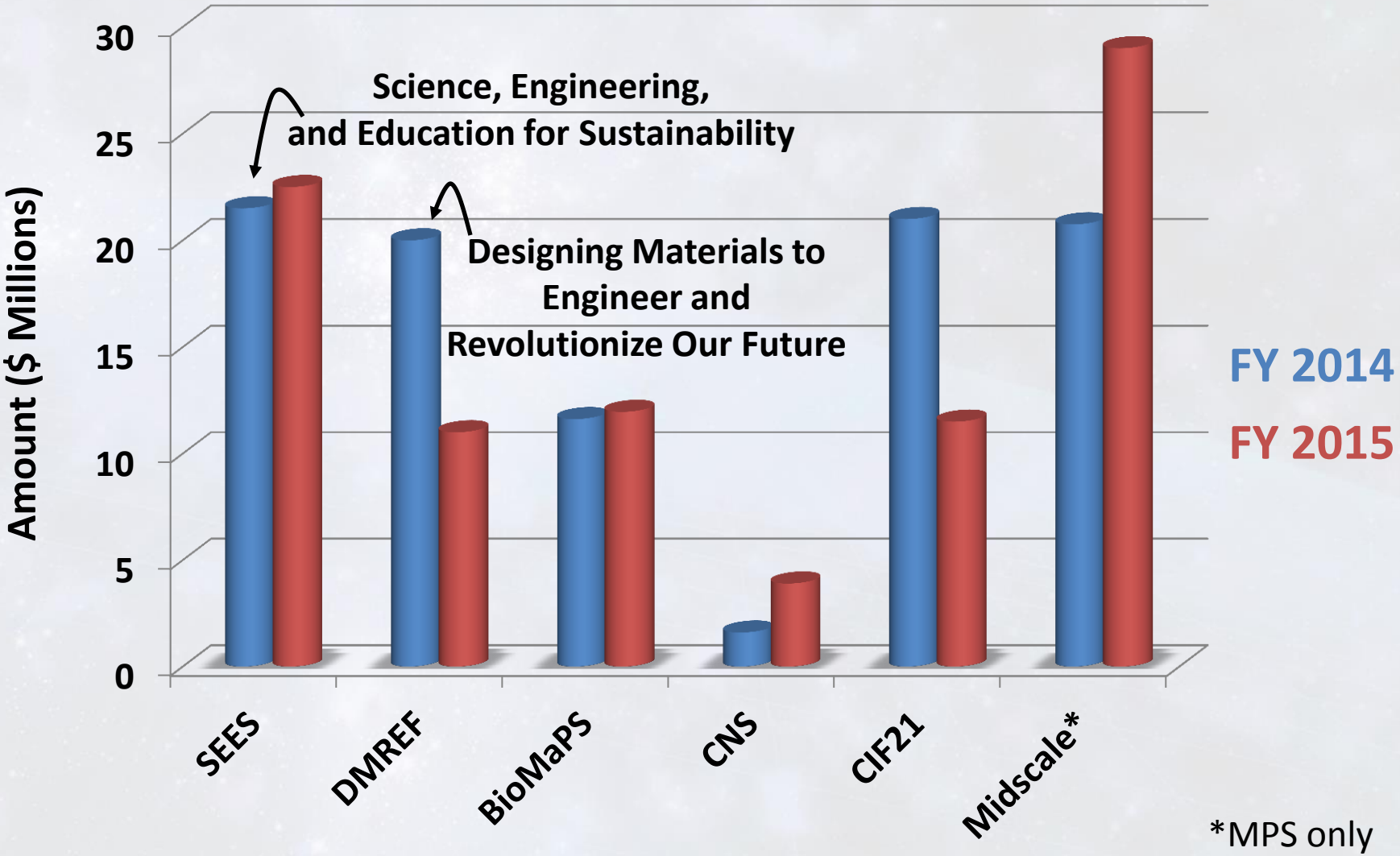


MPS Budgets

FY 2012 $ 1309 M → (−4.5%) → **FY 2013** $ 1250 M → (+4.0%) → **FY 2014** $ 1300 M (estimate) → (-0.3%) → **FY 2015** $ 1296 M (request)



Selected MPS Investments



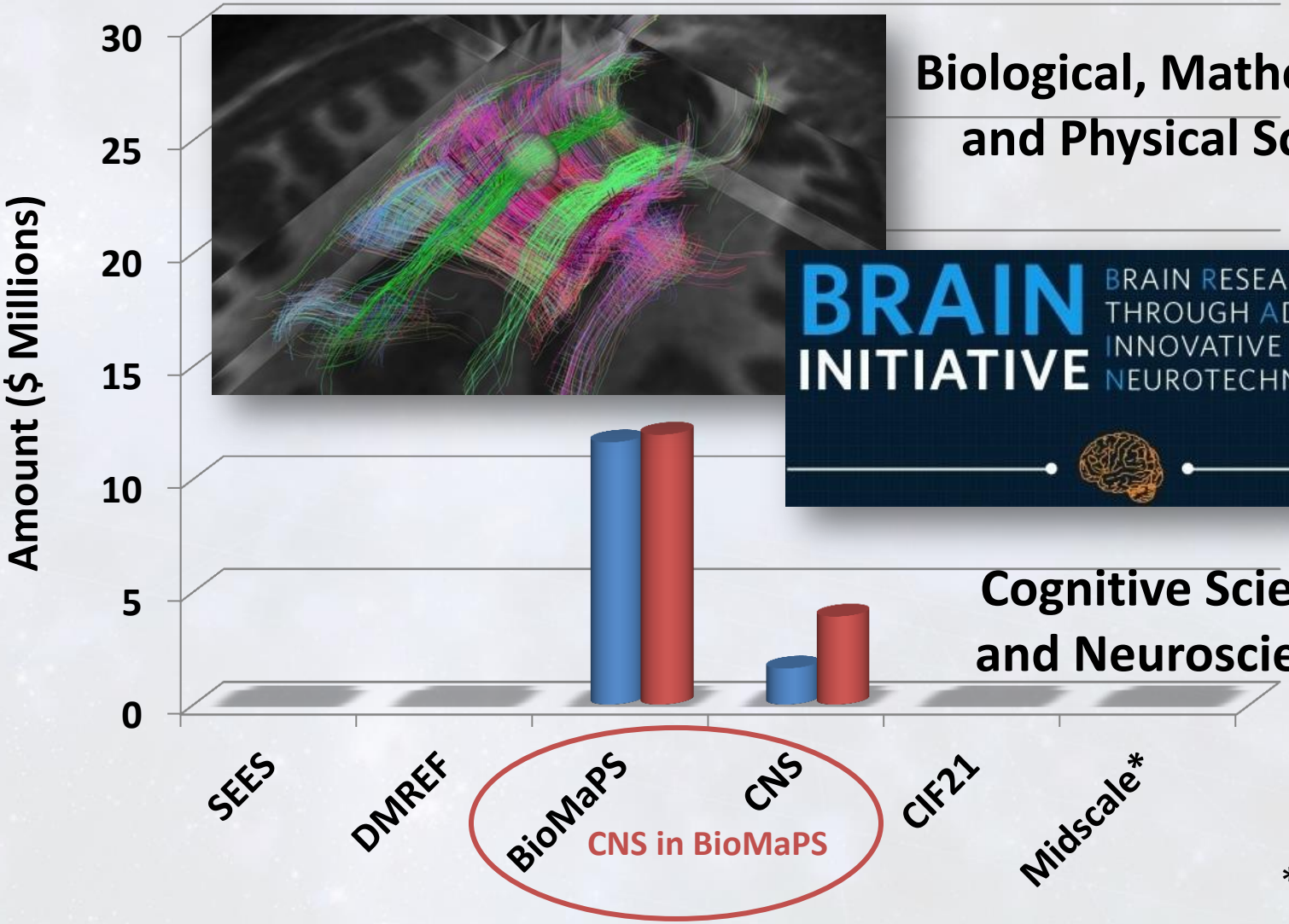
*MPS only

Selected MPS Investments

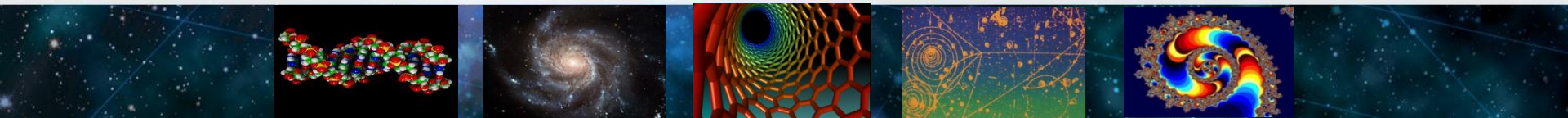
Biological, Mathematical, and Physical Sciences

BRAIN INITIATIVE
BRAIN RESEARCH THROUGH ADVANCING INNOVATIVE NEUROTECHNOLOGIES

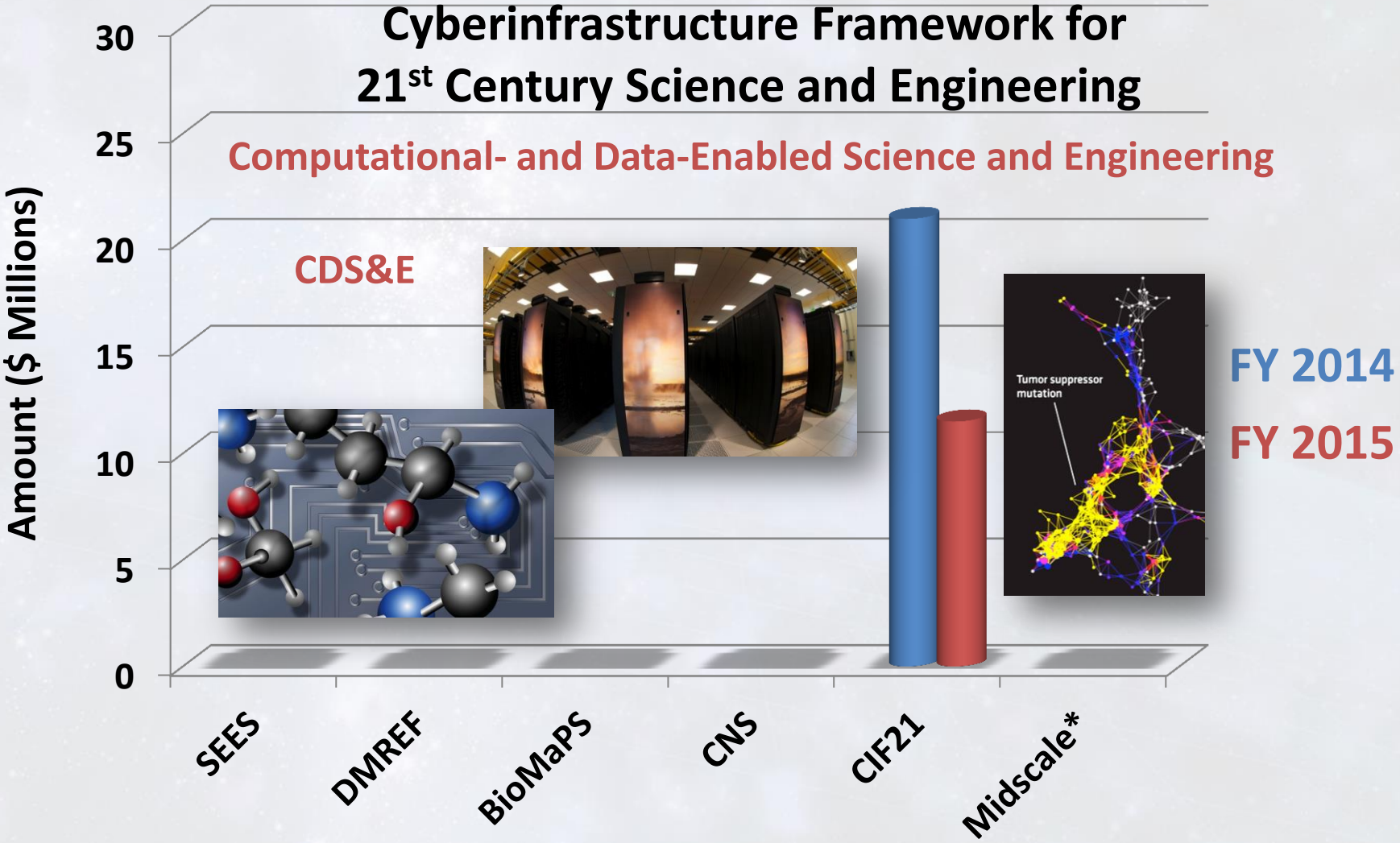
Cognitive Science and Neuroscience



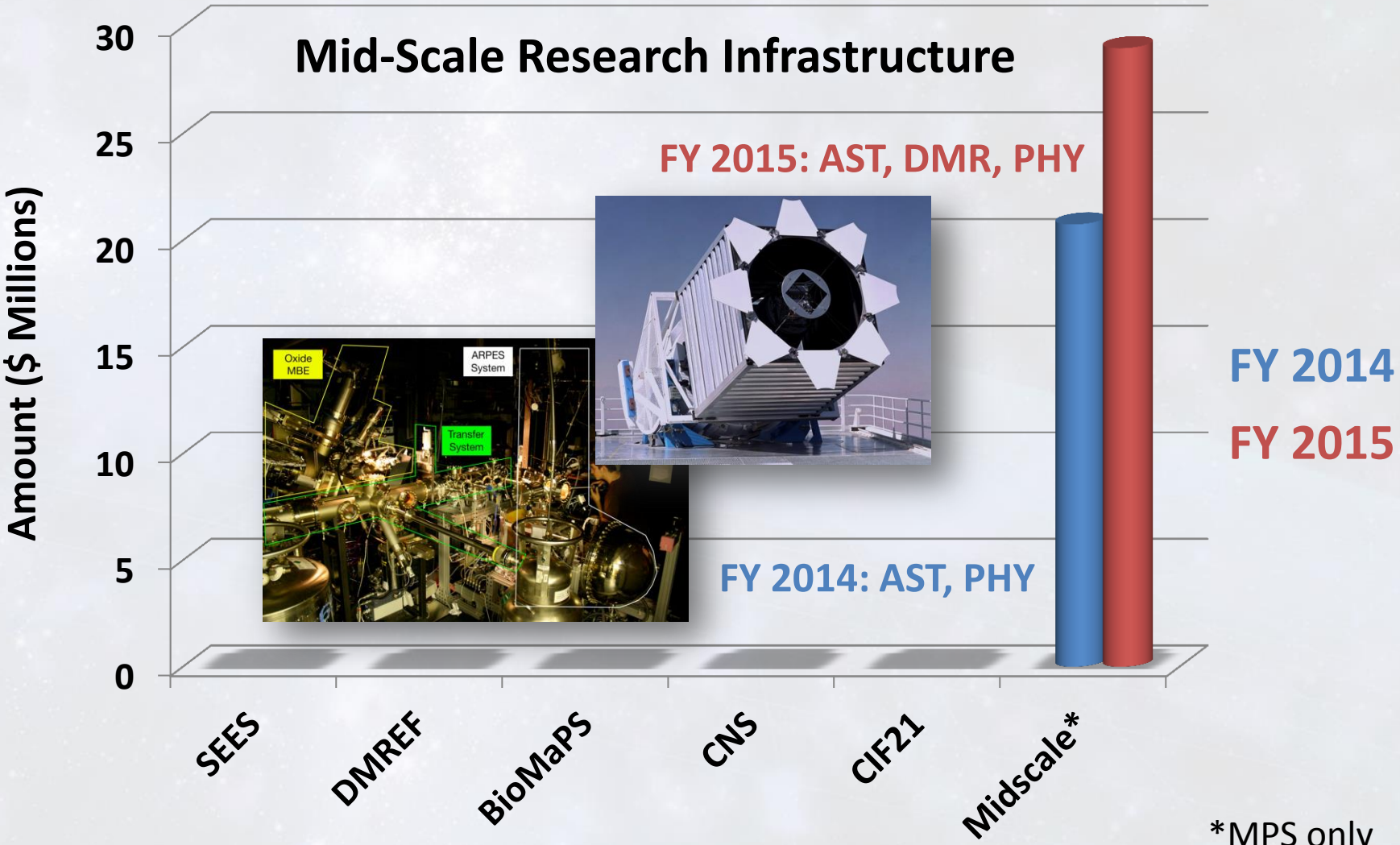
*MPS only



Selected MPS Investments



Selected MPS Investments



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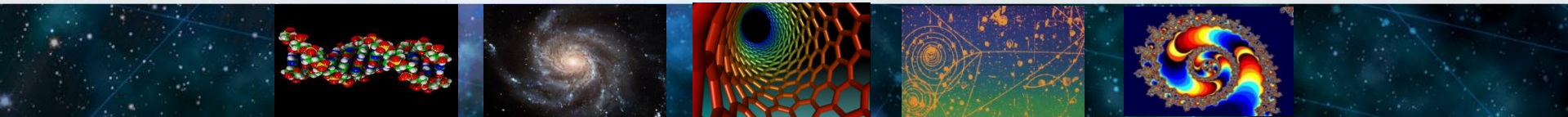
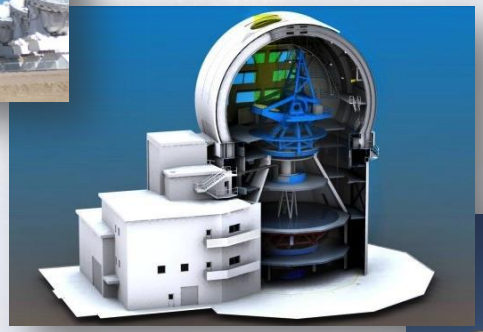


MPS-Supports Multi-user Facilities

ALMA

Gemini South

Blanco

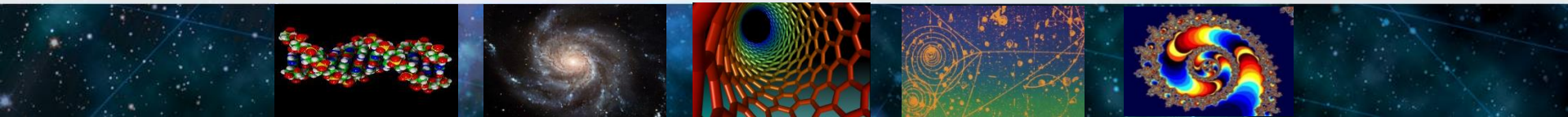


DKIST (ATST)

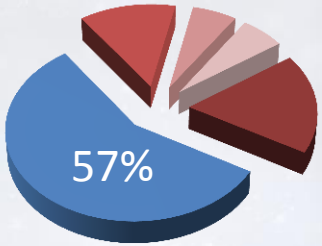
IceCube

NHMFL

LIGO



Two Different Budget Lines for Facilities

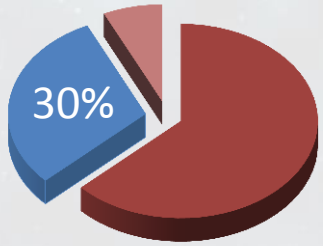


AST

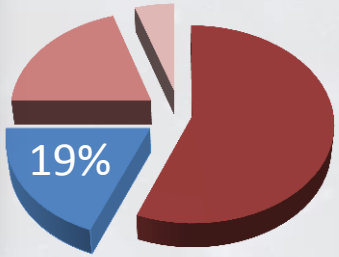
Operations (R&RA)

ALMA

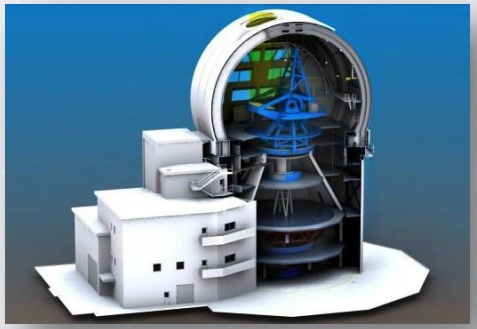
IceCube



PHY

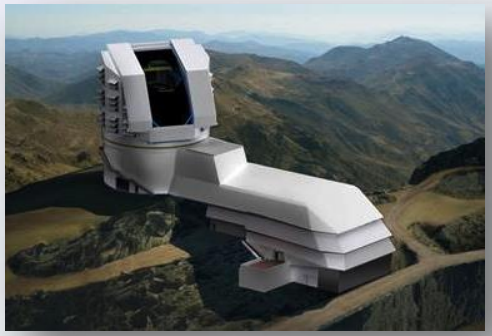


DMR

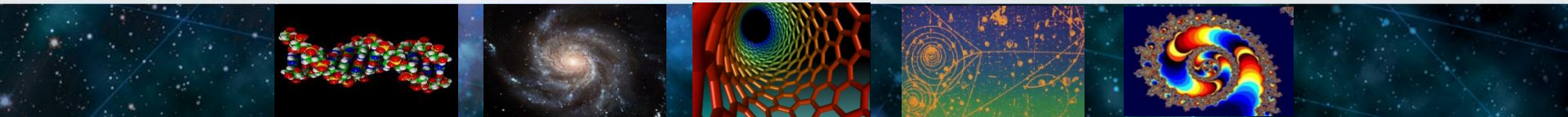


DKIST

Major Research Equipment and Facilities Construction (MREFC)



LSST



Helping Fill the STEM Pipeline Through MPS Research

CAREER
Young Teacher-Scholars

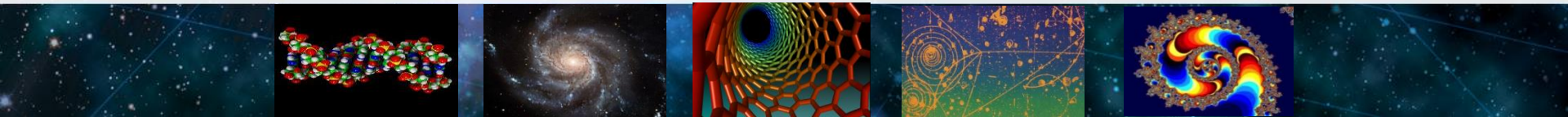
	FY 2014 Estimate	FY2015 Request
MPS	$ 65M	$ 66M
NSF	$ 210M	$ 213M

31% of CAREER funding from MPS

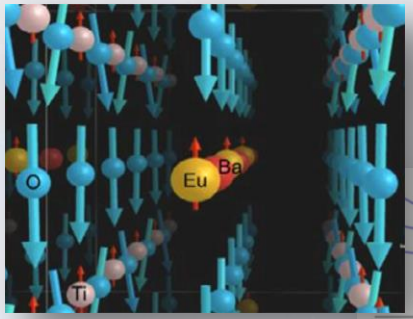
Research Experiences for Undergraduates (REU)
Undergraduate Research Programs

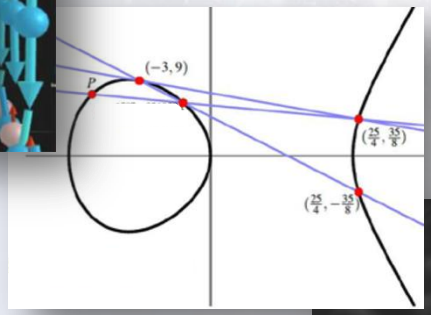
	FY 2014 Estimate	FY2015 Request
MPS	$ 22.4M	$ 21.2M
NSF	$ 75.3M	$ 75.1M

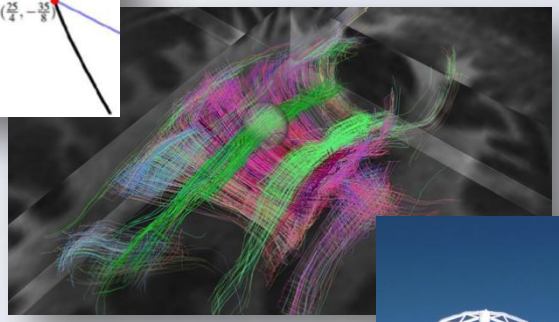
28% of REU funding from MPS



Fundamental Research in the Mathematical and Physical Sciences





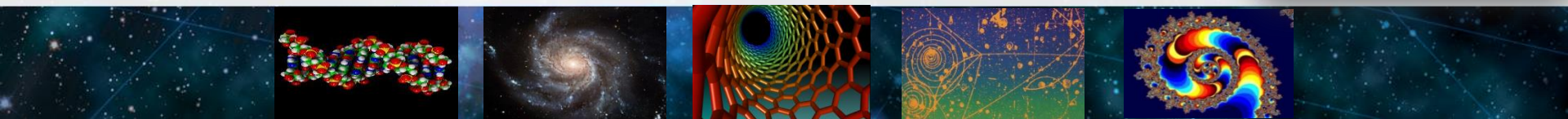


Advancing Discovery

Building Blocks for Innovation

Forefront Facilities

Inspiring the Next Generation



Personnel and Plans

Budget

Facilities

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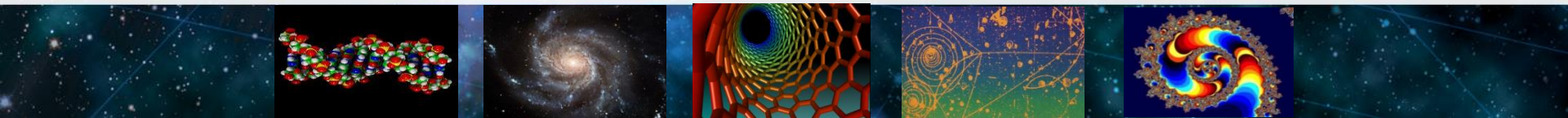


Transparency and Accountability: The Public Face of NSF

Titles

Clear, Concise, Cute

Good Vibrations: Making Molecules Boogie

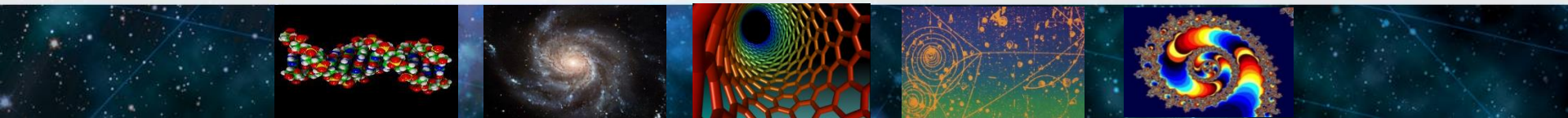
Vibrational Control of Chemical Reactions

Abstracts (Two Parts)

A Technical Description

A Non-technical Description for the Educated Reader (Not a Scientist or Engineer)

These parts do not necessarily map to "Broader Impacts" and "Intellectual Merit"



Transparency and Accountability: The NSF Portfolio

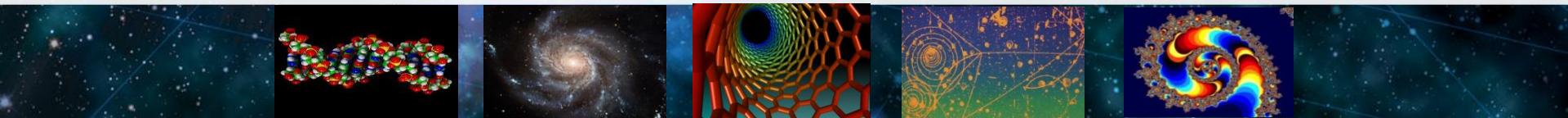
Individual Awards Build a Picture

NSF-supported research at the level of
Programs
Divisions
Directorates
Foundation

Describe portfolios to external stakeholders

Transparency and Accountability Working Group

Thanks to Brad Keister, DDD PHY



Transparency and Accountability: The NSF Portfolio

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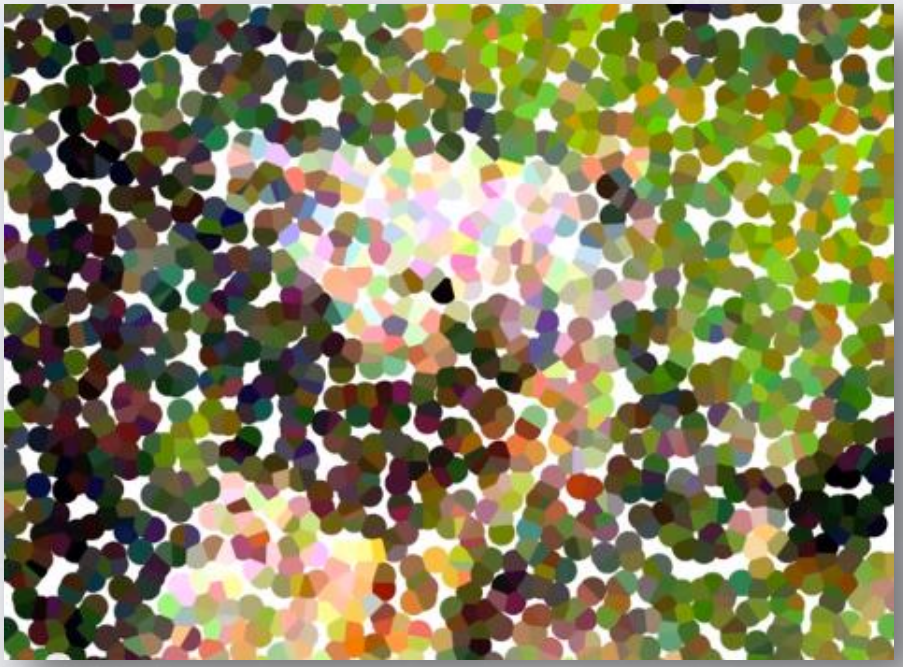
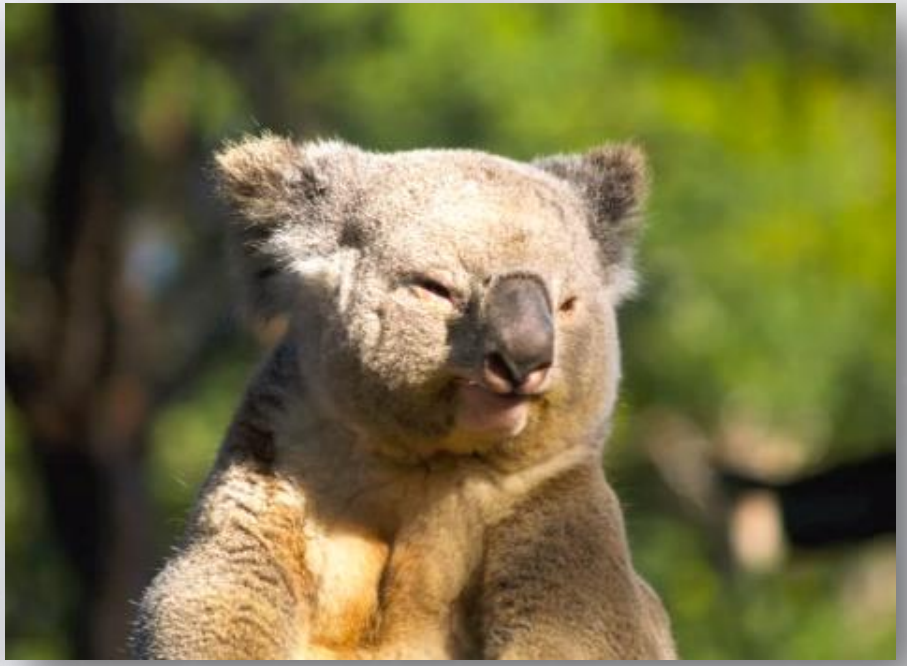
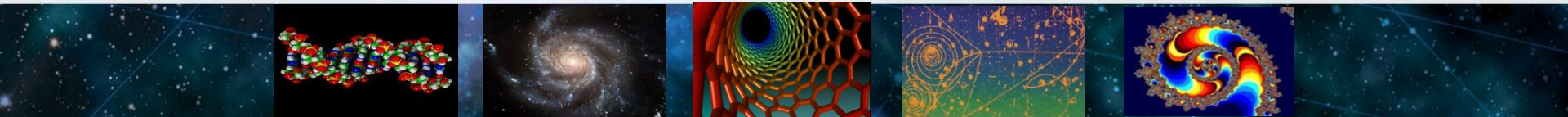




Ross Mannell: http://www.youtube.com/watch?v=QT5KtPoS-Tw



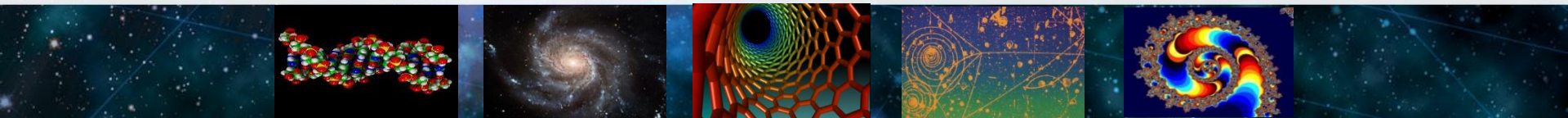
Personnel and Plans

Budget

Facilities

Program Updates

Agenda



Highlights for Today

Joint Meeting with Advisory Committee for Cyberinfrastructure ✓

State of the Directorate ✓

MPSAC Subcommittee Reports 50

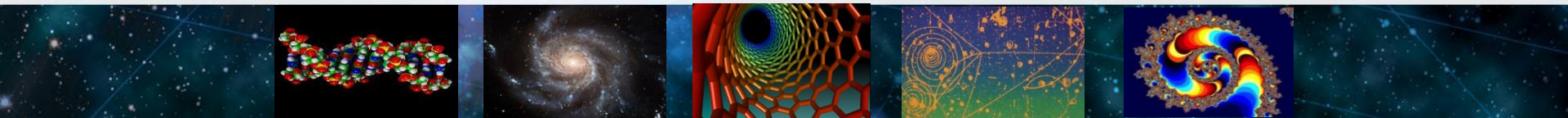
Stats NSF

Food Security

Meeting with the Director and Deputy Director 60

Dr. France Córdova, Director

Dr. Cora Marrett, Deputy Director



Highlights for Tomorrow

NSF Strategic Plan

Public Access to Publications and Data

MPSAC Subcommittee Reports

Optics and Photonics

Materials Instrumentation

Merit Review

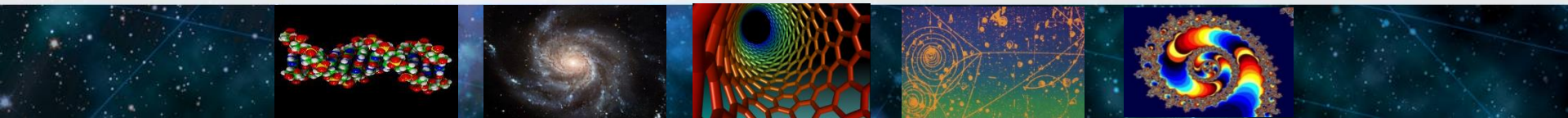
Part I: Issues, Lunch Breakout Group Discussions, Part II: Ideas

Reports

Committee on Equal Opportunity in Science and Engineering

Advisory Committee – International Science and Engineering

New Challenges and Subcommittees



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Focus on Discussion